Alpha-Particle Clustering from Expanding Self-Conjugate Nuclei within the Hartree-Fock-Bogoliubov Approach

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Alpha-Particle Clustering from Expanding Self-Conjugate Nuclei within the HFB Approach

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The nuclear equation of state is explored with the constrained HFB approach for self conjugate nuclei. It is found that beyond a certain low, more or less universal density, those nuclei spontaneously cluster into A/4 α particles with A the nucleon number. The energy at the threshold density increases linearly with the number of α particles as does the experimental threshold energy. Taking off the spurious c.o.m. energy of each α particle almost gives agreement between theory and experiment. The implications of these results with respect to α clustering and the nuclear EOS at low density are discussed.

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Introduction. Alpha-particle clustering in nuclei is highlighted by the famous Hoyle (0_2^+) state in ^{12}C at 7.65 MeV. This state, primordial for the ^{12}C production in the universe and, thus, for life, is believed since long to be in good approximation formed out of a weakly interacting gas of almost free α particles [1], [2], [3], [4]. Since these α particles are all in relative S-states, one can qualify this state as an α particle condensate [4] keeping in mind the limitations of this notion for finite systems with small numbers of particles. The research concerning this state has known a very vivid revival since about ten years when the hypothesis of the possible existence of α condensates in nuclei was formulated for the first time [4]. The investigations are now extending to heavier self-conjugate nuclei. On the forefront is ^{16}O where theoretical investigations predict that the 6-th 0^+ state at 15.1 MeV is an analogue of the Hoyle state but with four α particles instead of three [5]. Similarities between the three α and the four α cases are, indeed, being found experimentally [6]. The particularity of those α particle condensate states is that they are spatially extended [7], i.e., at a low average density of $\rho \sim \rho_{eq}/3 - \rho_{eq}/4$ with ρ_{eq} the average density at equilibrium of the nucleus. In this sense the α condensate states can be considered as a continuation of the structure of ^{8}Be which consists of two well identifiable, separate, weakly interacting α particles with average density in the just mentioned range [8]. On the other hand it is also well known that low density nuclear matter is unstable against cluster formation, mainly α particles [9], [10]. Theoretical predictions give a critical temperature for macroscopic α condensation as high as $T_c^\alpha \sim 7 - 8$ MeV at low densities [12]. From this fact, it can be inferred that the Hoyle state and possible heavier Hoyle analogue states are precursor states of a macroscopic α condensate phase, very much in analogy to neutron pairing in finite nuclei being a precursor to neutron superfluidity in neutron stars.

The microscopic description of α condensates in heavier nα nuclei naturally becomes more and more difficult and it seems at present impossible to describe, e.g., the clusterization of ^{40}Ca into ten α's based on a forty nucleon α cluster wave function as it may, e.g., be given by the THSR wave function [13]. On the other hand, certain 3D Hartree-Fock (HF) and Hartree-Fock-Bogoliubov (HFB) calculations of nuclei have recently shown that these mean field approaches can manifest cluster formation [14], [15], [16]. In this work, we concentrate within the HFB framework, using the Gogny D1S interaction, on constraining the radius of self-conjugate nuclei to larger and larger values, i.e., to lower and lower nuclear densities. In this way, we prevent a transition to strong deformation which would favor clusterization into binaries. Thus, expanding the nucleus, at a critical low density and because of the 3D nature of the code, the system will spontaneously cluster into α particles, eventually also into a heavier compact core with an α gas around it and other cluster formations. Those α particles do, of course, not form a condensate but rather build a lattice. This hinges on the fact that the α's have not the possibility to move freely with their center of mass (c.o.m.) coordinate in these HF or HFB calculations. The advantage of the mean field approach is that it can produce many α's in various configurations, still being entirely microscopic. So, qualitatively, the transition of an expanding nucleus passing from the homogeneous density distribution of a Fermi gas (HF) to clusterization can be studied within the mean field approach giving precious insights into the clusterization phenomenon in general and into the formation of α gas phases in particular. For example, as we will show, the energy of the system as a function of

the radius first raises from its equilibrium position going over a barrier and entering the cluster phase at around a density $\rho = \rho_{eq}/3$. This feature is of quite some interest as will be discussed below. Tracing the energy at this density as a function of the number n of α particles, i.e., as a function of the nucleon number A in case the whole nucleus disintegrates into α's, we find a perspicuous linear behavior with n. The slope of the experimental n-α threshold energies is quite a bit smaller than this theoretical 'threshold' curve but it also follows a straight line with about 7.6 MeV extra excitation energy per α. This stronger slope of our mean field results is due to the fact that, as already mentioned, the centers of the α's are spatially frozen in mean field. In order to correct, we follow a heuristic procedure. We perform an HFB calculation of ^{8}Be and constrain the distance between the two forming α's so that they are well separated. About 14 MeV are then missing to get twice the binding energy of a single α particle. We attribute this lack of binding to spurious c.o.m. motion of each α not being correctly treated. Of course, the total kinetic energy is subtracted from the Hamiltonian in all our calculations but if clusters or fragments are well formed, they develop their own spurious c.o.m. motion which should be taken away. So for ^{8}Be we have $\sim$ 7 MeV extra binding per α particle. We make the hypothesis that this number stays about the same, even in cases with more α particles.

Formalism and Results. Since the constrained HFB theory is extensively explained in the literature [17–20], we here only give the absolute minimum of formalism. We minimize the HFB ground state energy using the Gogny D1S [20] interaction in constraining the radius of the nucleus, that is

$$E^{\rm HFB} = \langle {\rm HFB}|H - \lambda r^2|{\rm HFB}\rangle / \langle {\rm HFB}|{\rm HFB}\rangle, \qquad (1)$$

where r is the radius. λ is obtained in such way that $\langle {\rm HFB}|r^2|{\rm HFB}\rangle/\langle {\rm HFB} = r_0^2$. Therefore, choosing values for r_0 $<$ or $>$ r_{GS}, where r_{GS} is the radius of the ground state, compresses or dilutes the nucleus. In the forthcoming, we treat all nuclei in spherical geometry, even though HFB may sometimes yield a deformed solution at the equilibrium position. Since we are interested in the low density (large radius) regime, it does not matter what is precisely the configuration at the absolute minimum. It should, however, be stressed that our 3D numerical code allows to take on any cluster configuration, if this is energetically favorable but on average the system stays spherical. For our study, we consider the selfconjugate N=Z nuclei up to ^{40}Ca. Let us first show the equation of state for the energy per particle as a function of density. Expanding (or compressing) a finite spherical nucleus yields, of course, not the usual equation of state as in infinite nuclear matter, since besides the bulk also surface and Coulomb energies together with the quantal shell corrections are involved. Therefore, this equation of state which

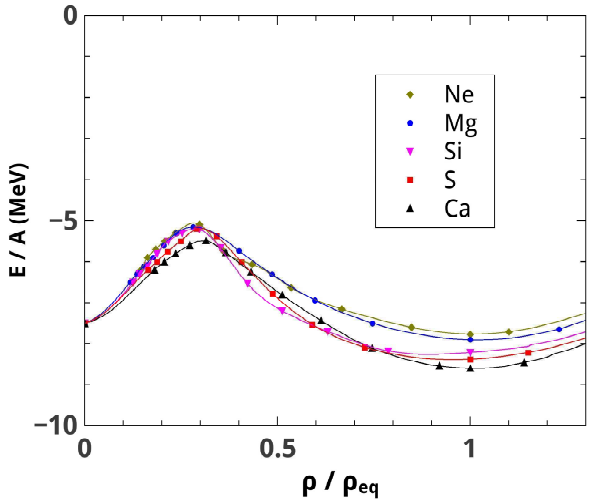

FIG. 1: (Color online) Equation of state for a choice of self-conjugate nuclei (EOS-A) as a function of average density scaled by the one at equilibrium, see text for detailed definition.

we want to call EOS-A slightly differs from nucleus to nucleus. Even for a given nucleus, in the low density region where clusters are formed, EOS-A may fluctuate, since in this region the energy surface has many different valleys leading to different cluster formations not very much different in energy. In which configuration the calculation gets trapped depends, e.g., on the step size of the expansion and other ingredients. In order to get a global view, we show in Fig. 1 the different EOS-A for various n-α nuclei superposed. With this, we want to put into evidence the general behavior of the nuclear equation of state at low densities when it goes over into an α particle configuration. As can be seen from Fig. 1, there is a clear tendency that the EOS-A goes as a function of decreasing density over a maximum before reaching the zero density limit where the α particles are infinitely far apart and, therefore, the EOS-A reaches the theoretical value of an isolated α particle, i.e. -7.5 MeV (the theoretical value). Evidently the numerical HFB code cannot handle configurations with α particles very distant from one another. Therefore, we stopped the calculation, once the α particles are clearly separated what happens around $\rho \sim \rho_{eq}/5$ (see also the detailed figures below). In Fig. 1, we show as an artist view lines extrapolating down to zero density just to guide the eye. In the region $\rho/\rho_{eq} \sim 0.3$, we adiabatically switch on the contribution of $\sim$ 7 MeV of each α particle to take care of its spurious c.o.m. motion as already discussed. The existence of a maximum in the nuclear equation of state containing a gas of α particles on the low density side and a Fermi gas (HF) on the higher density side is not evident. It would mean that the α phase is in a meta-stable state. The transition to the Fermi gas

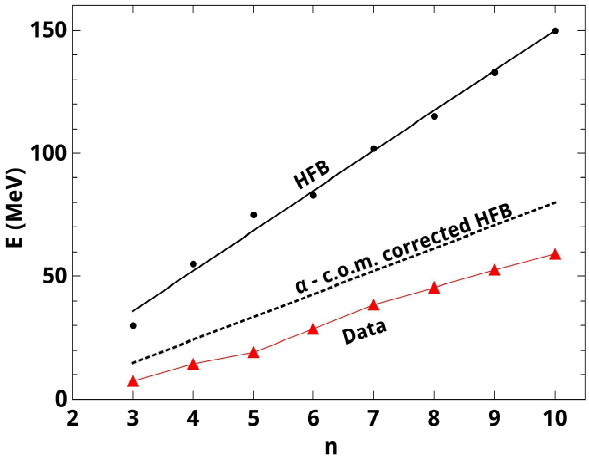

FIG. 2: (Color online) Threshold energies as a function of the number n of α particles. Triangles: experimental values; dots: values from HFB calculations, see text for precise definition; full line: best straight line fit to HFB results; broken line: alpha particle c.o.m. corrected HFB values.

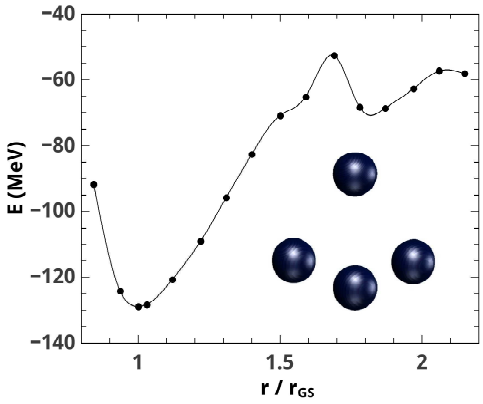

FIG. 3: (Color online) Total energy of ^{16}O as a function of the radius scaled with respect to the one of the ground state r_{GS}. At $< r > / < r >_{GS} = \sim 1.8$, we see the formation of a tetrahedron of four α particles. No c.o.m. correction for individual α's is applied here.

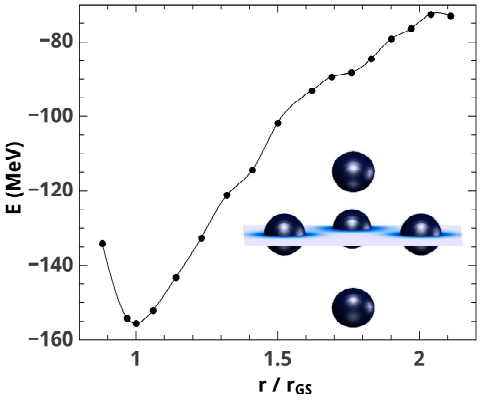

FIG. 4: (Color online) Same as Fig. 3 but for ^{20}Ne and the formation of five α's. The shaded plane serves only to show the three dimensionality of the figure.

configuration will be strongly different from the scenario when there is no barrier. This may be a question eventually of importance in compact stars where α particle phases may exist in the density-temperature space [21]. The present investigation seems to indicate the existence of a barrier about 2.5 MeV high but certainly more investigations have to be performed before a definite conclusion can be made. Let us also mention that there exists an infinite matter calculation considering α particles at low densities with a qualitatively similar result to ours [10].

Let us stress again that in a mean field calculation the α's are formed in a definite geometrical configuration. For example the four α's of ^{16}O form a tetrahedron and more complicated geometrical arrangements for heavier n α nuclei, see the figures below (for space reason, we will not show in this work the well known triangle configuration of ^{12}C, see, e.g., [11]). On the other hand, with the successful wave function of Tohsaki, Horiuchi, Schuck, Röpke (THSR), e.g., the Hoyle state in ^{12}C is interpreted as consisting with 70 percent of three α's condensed with their c.o.m. motion in a 0S wave. To simulate this delocalization effect, we take off, as already mentioned, ~ 7 MeV per α particle from the total energy.

Defining $\rho = \rho_{eq}/3$ as the theoretical threshold for α formation, we display in Fig. 2 the energy progression with the number n of α particles at that density. It is seen that this progression is about linear with n, increasing by ~ 16 MeV per α particle. Taking off the 7 MeV of spurious c.o.m. energy for each α particle strongly improves the agreement with experiment, see the broken line in Fig. 2. The experimental threshold energies follow rather well a 7.6 MeV increase per α particle. It is, however, clear that this procedure can only yield a very rough estimate of the real situation. It is encouraging that the overall picture seems to be quite reasonable. Since it is clear by now that the α particles form a quantum gas rather than a crystal, see [22] where a Brink-type, i.e. crystal-like of approach is put into competition with the THSR approach with the latter the clear winner, it will be important for the future to find less heuristic ways to take off the spurious c.o.m. energies from the clusters, once they are formed in the mean field approach.

Let us finally show in some detail the various α cluster configurations obtained from our constrained HFB calculation. In Fig. 3, we present the ^{16}O case. As already mentioned, at around $\rho = \rho_{eq}/3$ a tetrahedron of four α particles is formed. Actually the transition

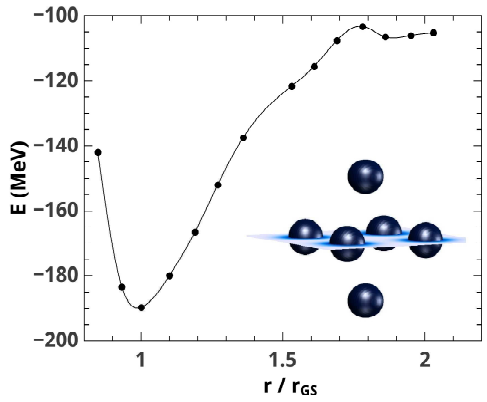

FIG. 5: (Color online) Same as Fig. 3 and Fig. 4 but for ^{24}Mg with six α's.

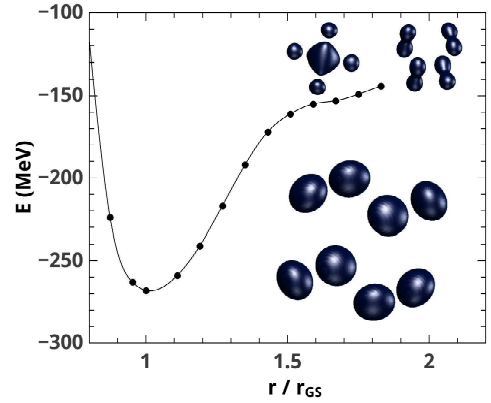

FIG. 6: (Color online) Same as Fig.3 but for ^{32}S with eight α's. Also configurations with four ^{8}Be's and a ^{16}O surrounded by four α's are shown.

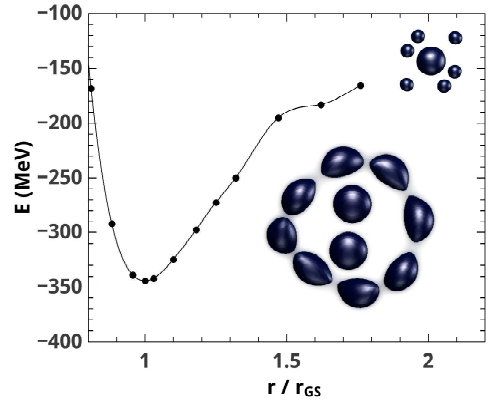

FIG. 7: (Color online) Same as Fig.3 but for ^{40}Ca with ten α's. Also configurations with a ^{16}O surrounded by six α's is shown

to the cluster state is quite abrupt. In Fig. 4, we show the ^{20}Ne case with a similar scenario and in Fig. 5 the ^{24}Mg case, in Fig. 6 ^{32}S and in Fig. 7 ^{40}Ca. Going to the heavier systems, it becomes more and more difficult to disrupt the system into α particles only. For example we show a four ^{8}Be configuration for ^{32}S and a ^{16}O plus six α case for ^{40}Ca. Many more cluster configurations can be obtained progressing, e.g. in smaller steps with the radius increment but for space reasons we cannot present this here. Let us only mention that we got an excited ^{36}Ar consisting out of three ^{12}C in a bent linear chain configuration. Also ^{48}Cr clustering into four ^{12}C has been found, and many configurations more.

Summary and Discussion. In this work, for the first time, a rather systematic study for quite a number of self-conjugate nuclei is presented within mean field theory concerning the formation of α particles when the nuclei are expanding that is, at low density. We here adopted a static approach revealing rich scenarios of α cluster configurations and other heavier clusters like ^{8}Be and ^{12}C. However, for the lighter nuclei α clusters are largely dominant. The mean field approach has the great advantage over other cluster models to be entirely microscopic employing a realistic energy density functional and to be able to describe the formation of quite a large number of α particles and eventually other clusters. It can cover within the same approach all density regions going in a continuous way from stable nuclei to highly excited ones at low density where the clusters form. It is found in this work that expanding an n-α nucleus the corresponding EOS-A goes over a maximum before reaching the asymptotic very low density limit of the α gas. This may be of importance in stabilizing an α phase. In principle there is no restriction for the mean field to produce any kind of shapes and clusters in which the systems want to go into. We also have checked that a single α particle is well described in HF with the Gogny force. Indeed, we have demonstrated in this work that that there can exist a great variety of rather surprising and unexpected cluster configurations when the nucleus is expanding.

On the theoretical side, the disadvantage of the mean field approach is that it fixes the clusters to certain spatial positions whereas it is predicted in recent work with the so-called THSR wave function that α particles rather form a degenerate quantum gas than a crystal [4, 22] (THSR). To overcome this drawback, we applied in this work a purely heuristic procedure in eliminating 'by hand' the spurious c.o.m. energy of each α particle. It is shown that in this way the theoretical threshold energies for n α's get rather close to the experimental values. The correct microscopic treatment of the spurious c.o.m. motion of clusters formed in a mean field approach remains an important task of nuclear many body physics for the future. For example, once the cluster formation is known from a mean field

calculation, one eventually may apply a Generator Coordinate Method to delocalize the clusters. Our work opens a variety of further investigations for the future. Most interesting is the cluster formation as a function of neutron excess. Also the generalization to time dependent HF will be full of information. Repeating our study with Relativistic Mean Field (RMF) may also be interesting, since it recently has been shown that RMF favors cluster formation [16]. We believe that the rich cluster scenarios found in this work are very inspiring and we hope that this will trigger more experimental and theoretical work on this line in the future.

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[1] H. Horiuchi, Prog. Theor. Phys. **51**, 1266 (1974); **53**, 447 (1975).
[2] M. Kamimura, Nucl. Phys. **A351**, 456 (1981).
[3] E. Uegaki, S. Okabe, Y. Abe, H. Tanaka, Prog. Theor. Phys. **57**, 1262 (1977); **59**, 1031 (1978); **62**, 1621 (1979).
[4] A. Tohsaki, H. Horiuchi, P. Schuck, G. Röpke, Phys. Rev. Lett. **87**, 192501 (2001).
[5] Y. Funaki, T. Yamada, H. Horiuchi, G. Roepke, P. Schuck, Phys. Rev. Lett. **101**, 082502 (2008).
[6] M. Itoh et al., talk given at 10th Int. Conf. on Clustering Aspects of Nuclear Structure and Dynamics, Debrecen, Hungary, 2012, J. Phys.: Conf. Ser. **436**, 012006 (2013).
[7] Y. Funaki, A. Tohsaki, H. Horiuchi, P. Schuck, G. Roepke, Eur. Phys. J. **A28**, 259 (2006).
[8] R.B. Wiringa, S.C. Pieper, J. Carlson, V.R. Pandharipande, Phys. Rev. C **62**, 014001 (2000).
[9] G. Röpke, L. Münchow, H. Schulz, Nucl. Phys. **A379**, 536 (1982); G. Röpke, M. Schmidt, L. Münchow, H. Schulz, Nucl. Phys. **A399**, 587 (1983).
[10] H. Takemoto, M. Fukushima, S. Chiba, H. Horiuchi, Y. Akaishi, A. Tohsaki, Phys. Rev. C **69**, 035802 (2004).
[11] M. Chernykh, H. Feldmeier, T. Neff, P. von Neumann-Cosel, A. Richter, Phys. Rev. Lett. **98**, 032501 (2007).
[12] T. Sogo, R. Lazauskas, G. Roepke, P. Schuck, Phys. Rev. C **79**, 051301 (2009).
[13] A. Tohsaki, Frontiers of Physics Vol. **6**, 320 (2011).
[14] Y. Funaki, M. Girod, H. Horiuchi, G. Röpke, P. Schuck, A. Tohsaki, T. Yamada, J. Phys. G **37**, 064012 (2010).
[15] T.Ichikawa, J.A. Maruhn, N. Itagaki, S. Ohkubo, Phys. Rev. Lett. **107**, 112501 (2011); T.Ichikawa, J.A. Maruhn, N. Itagaki, K. Matsuyanagi, P.-G. Reinhard, S. Ohkubo, Phys. Rev. Lett. **109**, 232503 (2012).
[16] J.-P. Ebran, E. Khan, T. Niksic, D. Vretenar, Phys. Rev. C **87**, 044307 (2012); ibidem: Nature **487**, 341 (2012).
[17] M. Girod, and B. Grammaticos, Phys. Rev. C **27**, 2317 (1983).
[18] M.Girod, J.P.Delaroche, D.Gogny, J.F.Berger, Phys. Rev. Lett. **62**, 2452 (1989).
[19] P. Ring, P. Schuck, The Nuclear many Body Problem, Springer 1980.
[20] J. Dechargé and D. Gogny, Phys. Rev. C **21**, 1568 (1980); J.F. Berger, M. Girod, and D. Gogny, Comp. Phys. Comm. **63**, 365 (1991).
[21] H. Shen, H. Toki, K. Oyamatsu, K. Sumiyoshi, Prog. Theor. Phys. **100**, 1013 (1998).
[22] Bo Zhou, Y. Funaki, H. Horiuchi, Zhongzhou Ren, G. Roepke, P. Schuck, A. Tohsaki, Chang Xu, T. Yamada, Phys. Rev. Lett. **110**, 262501 (2013).